

Orthoformic acid, cyclic 2,2-dimethyltrimethylene ethyl ester
5783-79-9 | DTXSID20206542

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.81 days

Global applicability domain: Outside

Local applicability domain index: 2.35e-01

Confidence level: 8.12e-01

Nearest Neighbors from the Training Set

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2-Methylheptane

Measured: 12.5

Predicted: 3.99

Image not found

2-Methylhexane

Measured: 12.5

Predicted: 5.54

Image not found

2-Methyloctane

Measured: 40.7

Predicted: 4.23

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2,4-Dimethylheptane

Measured: 61.9

Predicted: 4.29